

REMARKS

Claims 1-72 are pending, and claims 1-36 and 55-72 have been withdrawn from consideration. The Examiner has rejected the remaining claims—claims 37-54. Applicant thanks the Examiner for the close attention to this matter, and respectfully submits that the claims are now in condition for allowance.

Rejections under 35 U.S.C. § 112, second paragraph

The Examiner rejected claims 38-54 under 35 U.S.C. § 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which Applicant regards as the invention. In particular, the Examiner noted that the claims lack proper antecedent basis for the phrase “computer readable medium.” Applicant respectfully submits that, in light of the amendment to independent claim 37 to recite a “computer readable medium,” the rejection should be withdrawn.

Rejections under 35 U.S.C. § 102

The Examiner rejected claims 37-54 under 35 U.S.C. § 102(b) as anticipated by Gronbech-Jensen et al (U.S. Pat. 5,553,004). Essentially, the rejection was for a matter of form because the Examiner believed the claim recited “non-functional descriptive matter,” which the Examiner would not consider as distinguishing the invention from the prior art. Applicant has amended claim 37 to address the Examiner's concern.

As amended, claim 37 recites a computer-readable medium having computer executable instructions for performing a method, and as such, recites patentable subject matter. *See, e.g., In re Beauregard*, 53 F.3d 1583, 35 USPQ2d 1383 (Fed. Cir. 1995). Claim 37 as amended does not simply recite “descriptive material stored on or employed by a machine.” Rather, the claim recites instructions for performing a method of receiving information relating to a metal ion to be simulated, and generating a representation of a metal ion having certain stated properties. As amended, claim 37 thus recites a functional and patentable combination. Claims 38-54 depend on claim 37, and recite additional features of the invention.

With these features considered, the claimed invention is clearly patentably distinct from Gronbech-Jensen et al. For example, amended claim 37 recites receiving information relating to a metal ion, and generating a representation of a metal ion that comprises a center atom having a van der Waals radius greater than zero linked to one or more dummy atoms having a van der Waals radius of about zero. The claim also recites that the overall charge of the metal ion is evenly distributed among the dummy atoms, wherein the center atom has a charge of zero.

Gronbech-Jensen et al. completely fails to disclose or suggest these features. That patent discusses a stochastic dynamical method for simulating the motion of a molecular system, through simulating the motion of atoms by evaluating first order force expressions for all the atoms over a series of time steps. *See* Gronbech-Jensen et al., Abstract; *id.* col. 7, line 57 to col. 10, line 28. The Gronbech-Jensen et al. patent does not disclose or even suggest operation on metal ions having particular van der Waals radii as specified in the pending claims. Rather, it discusses the application of its method generally to macromolecules such as proteins and amino acids, and focuses on simplifying the representation of particular force interactions in the molecules. *See, e.g.*, Gronbech-Jensen et al., col. 7, line 57 to col. 10, line 28 (describing the force model); col. 11, line 23 to col. 27, line 2 (discussing "Simulation of Protein Dynamics").

The Gronbech-Jensen et al. patent differs in additional respects from the dependent claims. For example, claims 38 and 39 recite the mass of the dummy atom, claims 40-44 recite the particular geometric locations of the dummy atoms, claims 44-49 recite the type of the metal ion, claims 50-51 recite the calculated energy of solvation of the metal ion, and claims 52-54 recite the charge of the dummy atom. The Gronbech-Jensen et al. patent fails to disclose or even suggest any of these additional features of the invention.

For these reasons, the Applicants respectfully submit that claims 37-54 are in condition for allowance.

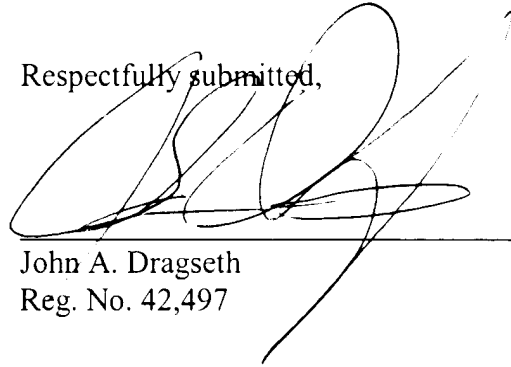
Attached is a marked-up version of the changes being made by the current amendment.

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Applicant asks that all claims be allowed. Please apply any charges or credits to Deposit Account No. 06-1050.

Respectfully submitted,



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Version with markings to show changes made

In the claims:

Claim 37 has been amended as follows:

-- 37. A computer readable medium having computer executable instructions for performing a method comprising:
receiving information relating to a metal ion to be simulated; and
generating [machine having a memory that contains data representing] a representation of a [simulated] metal ion [generated] by a molecular dynamics simulation, wherein said [simulated] representation of a metal ion comprises a center atom having a van der Waals radius greater than zero covalently linked to one or more dummy atoms having a van der Waals radius of about zero, wherein the overall charge of said metal ion is evenly distributed among said dummy atoms and wherein said center atom has a charge of zero. --

PENDING CLAIMS:

-- 37. A computer readable medium having computer executable instructions for performing a method comprising:
receiving information relating to a metal ion to be simulated; and
generating a representation of a metal ion by a molecular dynamics simulation, wherein said representation of a metal ion comprises a center atom having a van der Waals radius greater than zero covalently linked to one or more dummy atoms having a van der Waals radius of about zero, wherein the overall charge of said metal ion is evenly distributed among said dummy atoms and wherein said center atom has a charge of zero.

38. The computer readable medium of claim 37 wherein said dummy atom has a mass of about 0.1 g/mol.

39. The computer readable medium of claim 37 wherein said dummy atom has a mass greater than about 0.1 g/mol.
40. The computer readable medium of claim 37 wherein said dummy atoms are located at the apices of a polyhedron.
41. The computer readable medium of claim 40 wherein said center atom is located at the center of said polyhedron.
42. The computer readable medium of claim 40 wherein said polyhedron is selected from the group consisting of trigonal, tetrahedron, pentahedron, hexagonal, septagonal, and octahedral.
43. The computer readable medium of claim 41 wherein said polyhedron is a tetrahedron.
44. The computer readable medium of claim 37 wherein said metal ion is selected from a main group metal or transition metal.
45. The computer readable medium of claim 37 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.
46. The computer readable medium of claim 37 wherein said metal ion is zinc.
47. The computer readable medium of claim 41 wherein said metal ion is zinc.
48. The computer readable medium of claim 37 wherein said metal ion is magnesium.

49. The computer readable medium of claim 37 wherein said metal ion is calcium.
50. The computer readable medium of claim 37 wherein said metal ion has a calculated energy of solvation about equal to an experimentally determined energy of solvation for said metal ion.
51. The computer readable medium of claim 50 wherein said calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.
52. The computer readable medium of claim 37 wherein said dummy atom has a charge of about 0.5.
53. The computer readable medium of claim 37 wherein said dummy atom has a charge of about 0.3333.
54. The computer readable medium of claim 37 wherein said dummy atom has a charge ranging from about +0.1 to about +3.